Kubo effect

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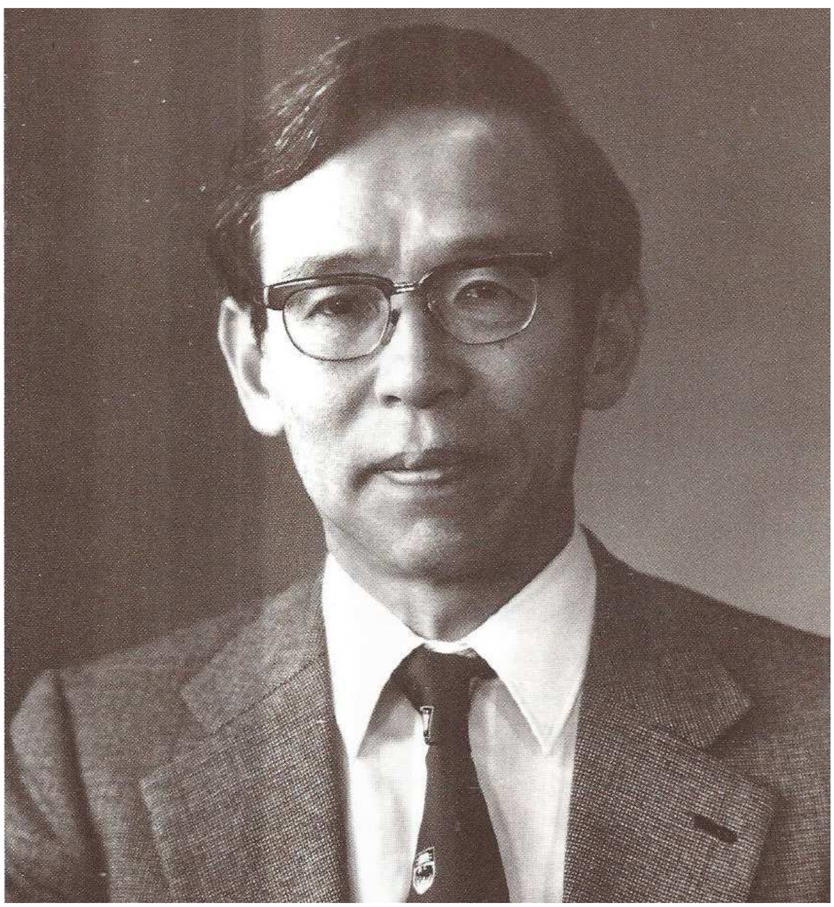
(Date: September 27, 2016)

Ryogo Kubo (February 15, 1920 – March 31, 1995) was a Japanese mathematical physicist, best known for his works in statistical physics and non-equilibrium statistical mechanics. In the early 1950s, Kubo transformed research into the linear response properties of near-equilibrium condensed-matter systems, in particular the understanding of electron transport and conductivity, through the Kubo formalism, a Green's function approach to linear response theory for quantum systems. In 1977 Ryogo Kubo was awarded the Boltzmann Medal *for his contributions to the theory of non-equilibrium statistical mechanics, and to the theory of fluctuation phenomena*. He is cited particularly for his work in the establishment of the basic relations between transport coefficients and equilibrium time correlation functions: relations with which his name is generally associated.

https://en.wikipedia.org/wiki/Ryogo_Kubo



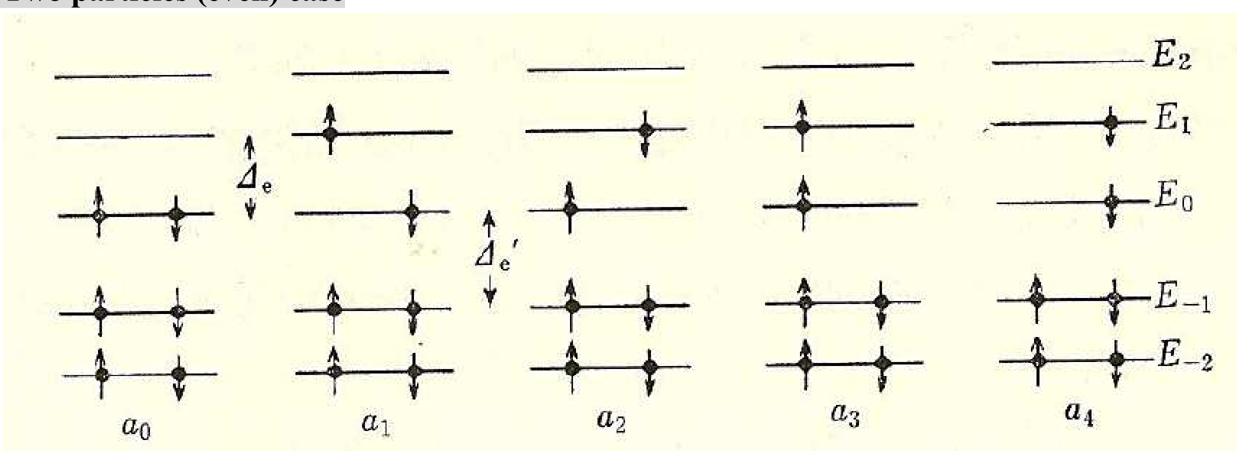
Prof. Ryogo Kubo (from Selected Papers of Professor Ryogo Kubo on the Occasion of his Sixtieth Birthday (Syokabo, 1980).

The physics of the mesoscopic system started with the theory of metal fine particles, which was first proposed by Prof. Ryogo Kubo. When electrons are enclosed in a system with finite size, the energy levels of electron becomes discrete. The separation of the energy levels is typically larger than the thermal energy. So the physical properties of the metallic fine particles may be rather different from those of bulk system where the energy spectrum is continuous. The number of electrons is on the order of 10^5 for fine particles whose diameter is several 10 Å. Experimentally, such a difference may be experimentally observed in the susceptibility and heat capacity measurements. For simplicity, there is no degeneracy in the discrete energy levels.

According to Kubo's theory, the number of spins in the particles strongly affects the magnetic properties, depending on whether it is even or odd. The statistical mechanics is discussed for two particles (even) and for one particle (odd). The susceptibility and heat capacity can be calculated from the method of canonical ensemble. We can show that the susceptibility shows the Curie law for the one particle system, and that it decreases with decreasing temperature and reduced to zero at low temperatures for the even particle system.

Kubo effect is a good exercise for the canonical ensemble.

1. Two particles (even) case



We consider a system of two particles.

The partition function for the two particles is given by

$$Z = \exp[-\beta(2\varepsilon_0)] + 4\exp[-\beta(\varepsilon_0 + \varepsilon_1)] + \exp[-\beta(2\varepsilon_1)]$$

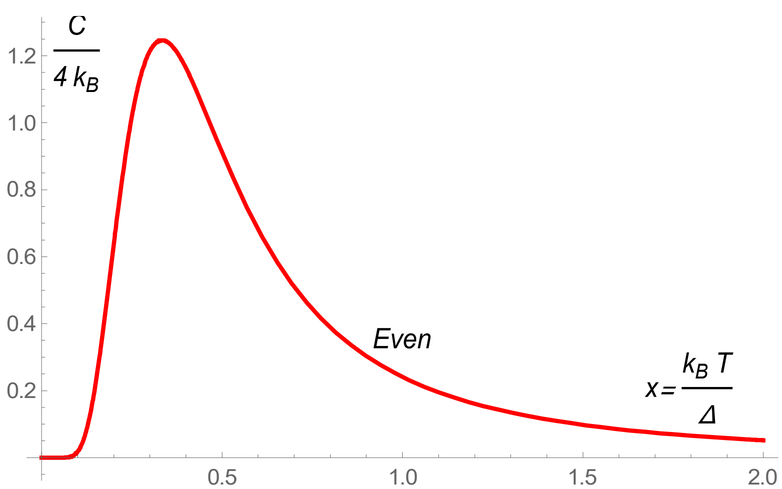
The average energy is

$$
\begin{aligned}
\langle E\rangle &= -\frac{\partial}{\partial\beta}\ln Z \\
&= \frac{2\varepsilon_0\exp[-\beta(2\varepsilon_0)]+4(\varepsilon_0+\varepsilon_1)\exp[-\beta(\varepsilon_0+\varepsilon_1)]+2\varepsilon_1\exp[-\beta(2\varepsilon_1)]}{\exp[-\beta(2\varepsilon_0)]+4\exp[-\beta(\varepsilon_0+\varepsilon_1)]+\exp[-\beta(2\varepsilon_1)]} \\
&= \frac{2\varepsilon_0+4(\varepsilon_0+\varepsilon_1)\exp[-\beta(\varepsilon_1-\varepsilon_0)]+2\varepsilon_1\exp[-2\beta(\varepsilon_1-\varepsilon_0)]}{1+4\exp[-\beta(\varepsilon_1-\varepsilon_0)]+\exp[-2\beta(\varepsilon_1-\varepsilon_0)]} \\
&\approx \frac{2\varepsilon_0+4(\varepsilon_0+\varepsilon_0)\exp[-\beta(\varepsilon_1-\varepsilon_0)]}{1+4\exp[-\beta(\varepsilon_1-\varepsilon_0)]} \\
&= 2\varepsilon_0+\frac{4\Delta e^{-\beta\Delta}}{1+4e^{-\beta\Delta}}
\end{aligned}
$$

where we neglect the term $\exp[-2\beta(\varepsilon_1-\varepsilon_0)]$ both in the denominator and numerator.
The heat capacity is

$$
C=\frac{\partial E}{\partial T}=\frac{\partial}{\partial T}\left(\frac{4\Delta e^{-\beta\Delta}}{1+4e^{-\beta\Delta}}\right)=4k_B\frac{e^{\beta\Delta}}{(4+e^{\beta\Delta})^2}(\beta\Delta)^2
$$

We make a plot of $C/(4k_B)$ as a function of $x=\frac{k_BT}{\Delta}$. This curve has a maximum (1.24645) at x = 0.333597.



The magnetic moment $\boldsymbol{\mu}$ of spin is given by

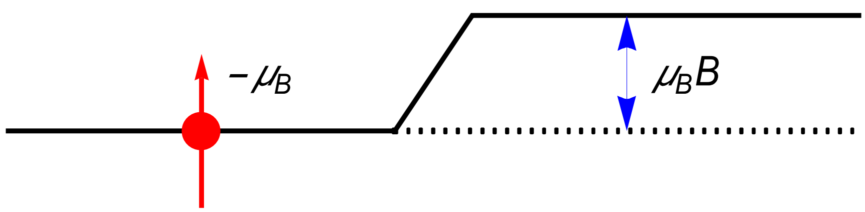
$$
\boldsymbol{\mu}=-\frac{2\mu_B}{\hbar}\boldsymbol{S},
$$

where μ_B is the Bohr magneton. In the presence of a magnetic field along the z axis, we have a Zeeman energy

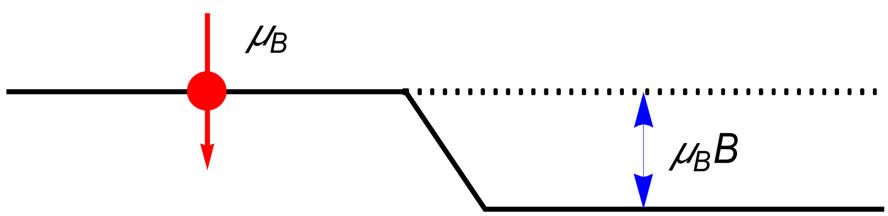
$$H_z = -\boldsymbol{\mu}\cdot\boldsymbol{B} = -\left(-\frac{2\mu_B}{\hbar}\boldsymbol{S}\right)\cdot\boldsymbol{B} = \frac{2\mu_B B}{\hbar}S_z = \frac{2\mu_B B}{\hbar}\frac{\hbar}{2}\sigma = \mu_B B\sigma\,,$$

where $S_z = \frac{\hbar}{2}\sigma_z$.

(a) Spin-up state:



(b) Spin-down state:



When the magnetic field is applied along the z axis, the partition function is

$$\begin{aligned}
Z(B) &= \exp[-\beta(2\varepsilon_0)] + 2\exp[-\beta(\varepsilon_0+\varepsilon_1)] + \exp[-\beta(2\varepsilon_1\ )] \\
&\quad + \exp[-\beta(\varepsilon_0+\varepsilon_1+2\mu_B B)] + \exp[-\beta(\varepsilon_0+\varepsilon_1-2\mu_B B)] \\
&= \exp[-\beta(\varepsilon_0+\varepsilon_1)]\{\exp(-2\beta\mu_B B)+\exp(2\beta\mu_B B)\} \\
&\quad + \exp[\beta(\varepsilon_1-\varepsilon_0)] + 2 + \exp[-\beta(\varepsilon_1-\varepsilon_0)]\} \\
&= \exp[-\beta(\varepsilon_0+\varepsilon_1)]\{2\cosh(\beta\mu_B B) + 2\cosh(\beta(\Delta)+2]
\end{aligned}$$

The average energy:

$$
\begin{aligned}
\langle E \rangle &= -\frac{\partial}{\partial \beta} \ln Z(B) \\
&= -\frac{1}{Z(B)} \frac{\partial}{\partial \beta} Z(B) \\
&= \frac{1}{Z(B)} [(2\varepsilon_0) \exp[-\beta(2\varepsilon_0)] + 2(\varepsilon_0 + \varepsilon_1) \exp[-\beta(\varepsilon_0 + \varepsilon_1)] + (2\varepsilon_1) \exp[-\beta(2\varepsilon_1)] \\
&\quad + (\varepsilon_0 + \varepsilon_1 + 2\mu_B B) \exp[-\beta(\varepsilon_0 + \varepsilon_1 + 2\mu_B B)] \\
&\quad + (\varepsilon_0 + \varepsilon_1 - 2\mu_B B) \exp[-\beta(\varepsilon_0 + \varepsilon_1 - 2\mu_B B)]]
\end{aligned}
$$

The average magnetization:

$$
\langle M \rangle = -\frac{\partial F}{\partial B} = -k_B T \frac{\partial}{\partial B} \ln Z = -k_B T \frac{1}{Z} \frac{\partial}{\partial B} Z = -\frac{1}{\beta} \frac{1}{Z} \frac{\partial}{\partial B} Z
$$

or

$$
\begin{aligned}
\langle M \rangle &= \frac{1}{Z} \{2\mu_B \exp[-\beta(\varepsilon_0 + \varepsilon_1 + 2\mu_B B)] - 2\mu_B \exp[-\beta(\varepsilon_0 + \varepsilon_1 - 2\mu_B B)]\} \\
&= \frac{-4\mu_B [\exp(2\beta\mu_B B) - \exp(-2\beta\mu_B B)]}{2\cosh(\beta\mu_B B) + 2\cosh(\beta(\Delta) + 2} \\
&= -\frac{2\mu_B \sinh(2\beta\mu_B B)}{\cosh(2\beta\mu_B B) + \cosh(\beta\Delta) + 1}
\end{aligned}
$$

In the weak limit of B,

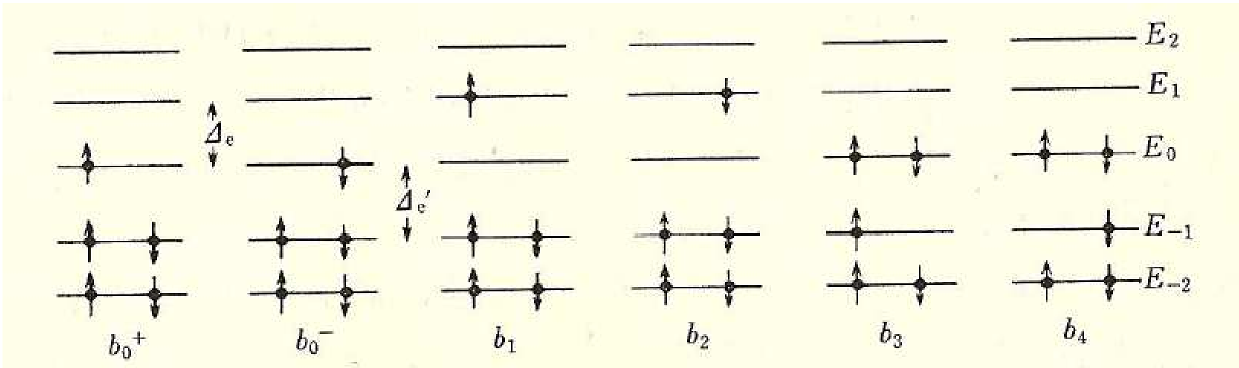
$$
\langle M \rangle \approx -\frac{4\mu_B{}^2 \beta B}{2 + \cosh(\beta\Delta)} \approx -\frac{8\mu_B{}^2 B}{k_B T} e^{-\beta\Delta}
$$

So the susceptibility

$$
\chi = \frac{\langle M \rangle}{B} = \frac{\mu_B{}^2}{k_B T} e^{-\beta\Delta}
$$

which tends to be reduced to zero at $T = 0$. It seems that two spins are antiferromagnetically coupled at low temperatures.

2. One particle case



We consider a system of one particle. Here we only consider the case of b_0^+, b_0^-, b_1, and b_2.

The partition function for the one particles is given by

$$Z = 2\exp(-\beta\varepsilon_0) + 2\exp(-\beta\varepsilon_1)$$

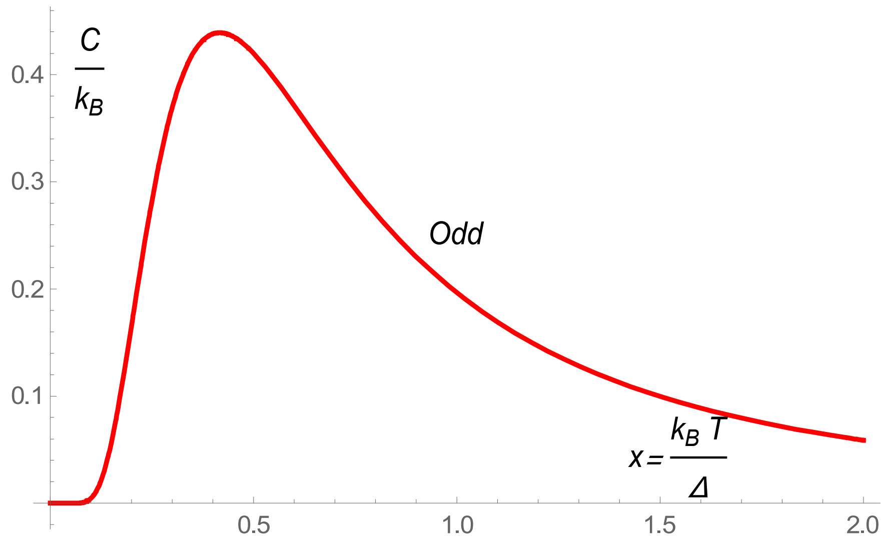
The average energy is

$$\begin{aligned}\langle E\rangle &= -\frac{\partial}{\partial\beta}\ln Z \\ &= \frac{\varepsilon_0\exp(-\beta\varepsilon_0) + \varepsilon_1\exp(-\beta\varepsilon_1)}{\exp(-\beta\varepsilon_0) + \exp(-\beta\varepsilon_1)} \\ &= \varepsilon_1 - \frac{\Delta}{1+e^{-\beta\Delta}}\end{aligned}$$

The heat capacity:

$$C = \frac{\partial E}{\partial T} = -\frac{\partial}{\partial T}\left(\frac{\Delta}{1+e^{-\beta\Delta}}\right) = k_B\frac{e^{\beta\Delta}}{(1+e^{\beta\Delta})^2}(\beta\Delta)^2$$

We make a plot of $C/(k_B)$ as a function of $x = \frac{k_B T}{\Delta}$. This curve has a maximum (0.439229) at x = 0.416778.



When the magnetic field is applied along the *z* axis, the partition function is

$$\begin{aligned} Z(B) &= \exp[-\beta(\varepsilon_0 + \mu_B B)] + \exp[-\beta(\varepsilon_0 - \mu_B B)] \\ &\quad + \exp[-\beta(\varepsilon_1 + \mu_B B)] + \exp[-\beta(\varepsilon_1 - \mu_B B)] \end{aligned}$$

The average magnetization:

$$\langle M \rangle = -\frac{\partial F}{\partial B} = -k_B T \frac{\partial}{\partial B} \ln Z = -k_B T \frac{1}{Z} \frac{\partial}{\partial B} Z = -\frac{1}{\beta} \frac{1}{Z} \frac{\partial}{\partial B} Z$$

$$\begin{aligned} \langle M \rangle &= -\frac{1}{\beta} \frac{1}{Z} \frac{\partial}{\partial B} Z \\ &= \frac{\mu_B}{Z} [\exp[-\beta(\varepsilon_0 + \mu_B B)] - \exp[-\beta(\varepsilon_0 - \mu_B B)] \\ &\quad + \exp[-\beta(\varepsilon_1 + \mu_B B)] - \exp[-\beta(\varepsilon_1 - \mu_B B)] \\ &= -\mu_B \frac{(1 + e^{-\beta\Delta})[\exp(\beta\mu_B B) - \exp(\beta\mu_B B)]}{(1 + e^{-\beta\Delta})[\exp(\beta\mu_B B) + \exp(-\beta\mu_B B)]} \\ &= -\mu_B \tanh(\beta\mu_B B) \end{aligned}$$

In the weak limit of magnetic field,

$$\langle M \rangle \approx -\frac{\mu_B{}^2 B}{k_B T} \qquad \text{or} \qquad \chi = \frac{\langle M \rangle}{B} = \frac{\mu_B{}^2}{k_B T}$$

showing the Curie law.

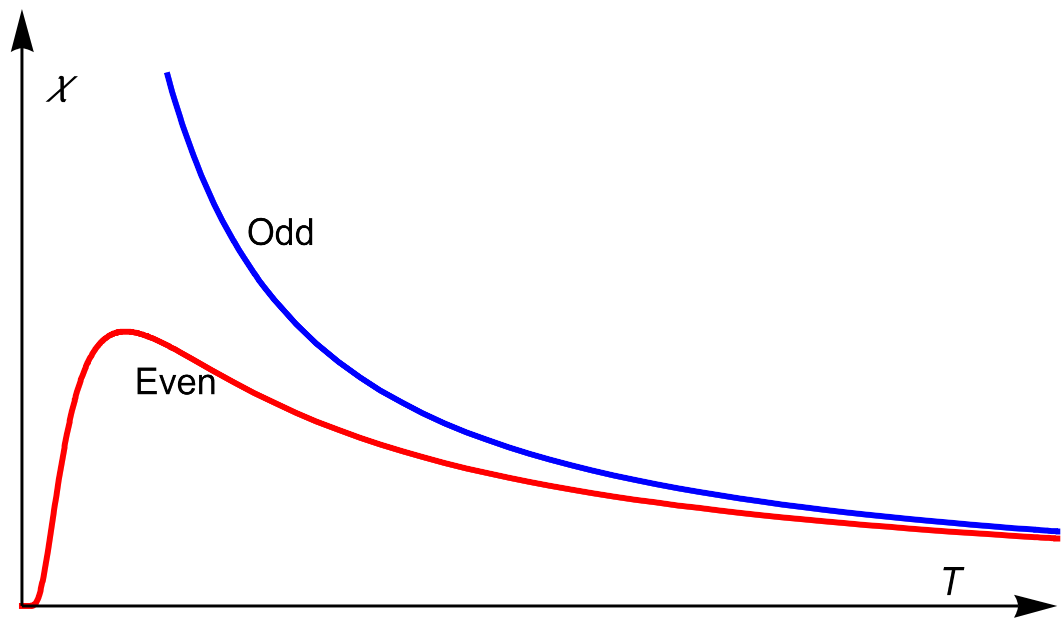


Fig. Susceptibility vs T for the even (2 particles) and odd (1 particle) systems.